

chain nodes :

1 3 4 5 12 15 17 18 19 20

ring nodes :

6 7 8 9 10 11

chain bonds :

1-12 3-4 3-12 4-5 5-8 15-17 17-18 18-19 18-20

ring bonds :

6-7 6-11 7-8 8-9 9-10 10-11

exact/norm bonds :

1-12 3-12 5-8 18-20

exact bonds :

3-4 4-5 15-17 17-18 18-19

normalized bonds :

6-7 6-11 7-8 8-9 9-10 10-11

isolated ring systems :

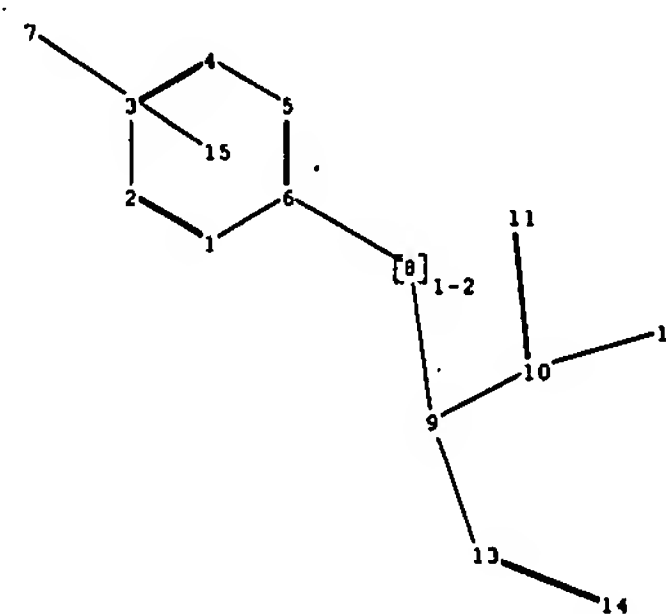
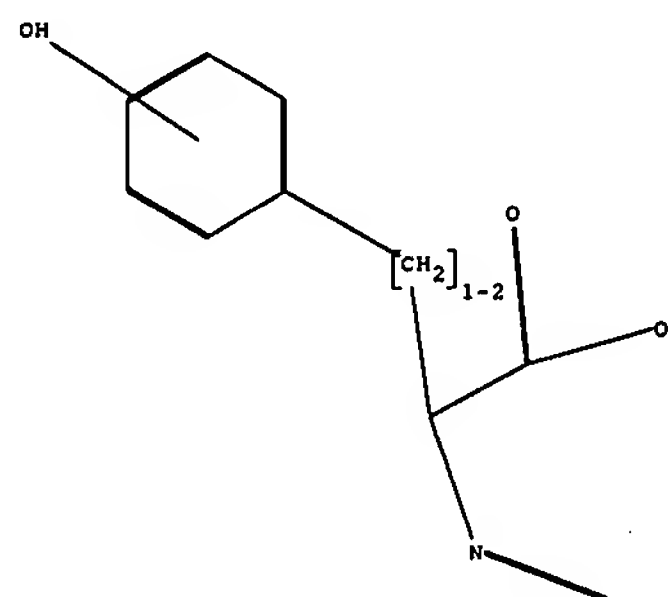
containing 6 :

Connectivity :

1:1 E exact RC ring/chain

Match level :

1:CLASS 3:CLASS 4:CLASS 5:CLASS 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 15:CLASS 16:Atom 17:CLASS 18:CLASS 19:CLASS 20:CLASS



chain nodes :

7 8 9 10 11 12 13 14

ring nodes :

1 2 3 4 5 6

chain bonds :

6-8 8-9 9-10 9-13 10-11 10-12 13-14

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

9-13 10-11 10-12 13-14

exact bonds :

6-8 8-9 9-10

normalized bonds :

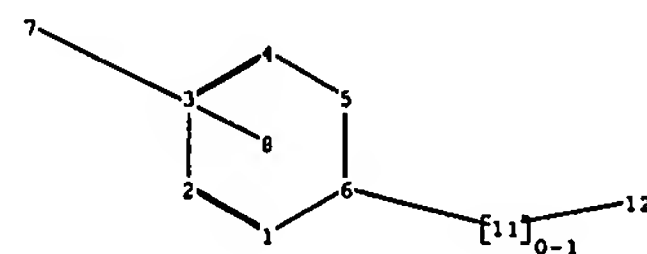
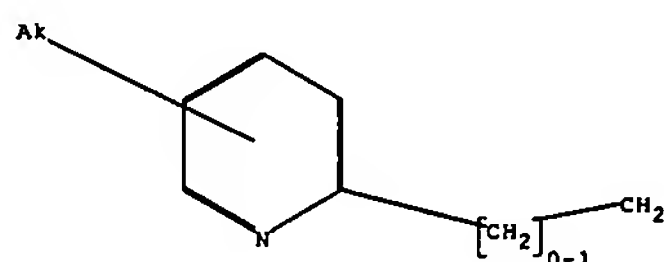
1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS
10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:Atom



chain nodes :

7 11 12

ring nodes :

1 2 3 4 5 6

chain bonds :

6-11 11-12

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact bonds :

6-11 11-12

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

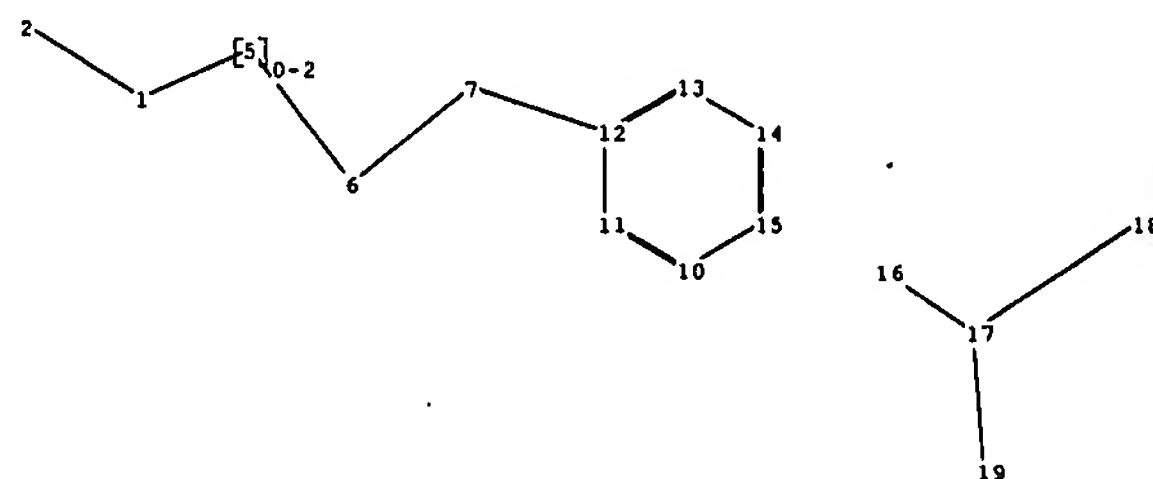
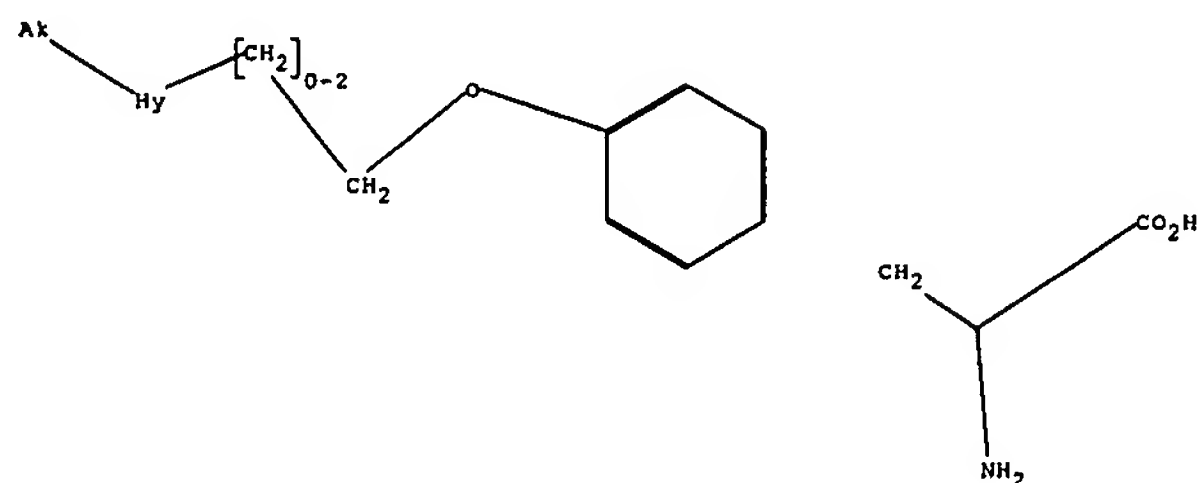
containing 1 :

Connectivity :

7:1 E exact RC ring/chain

Match level :

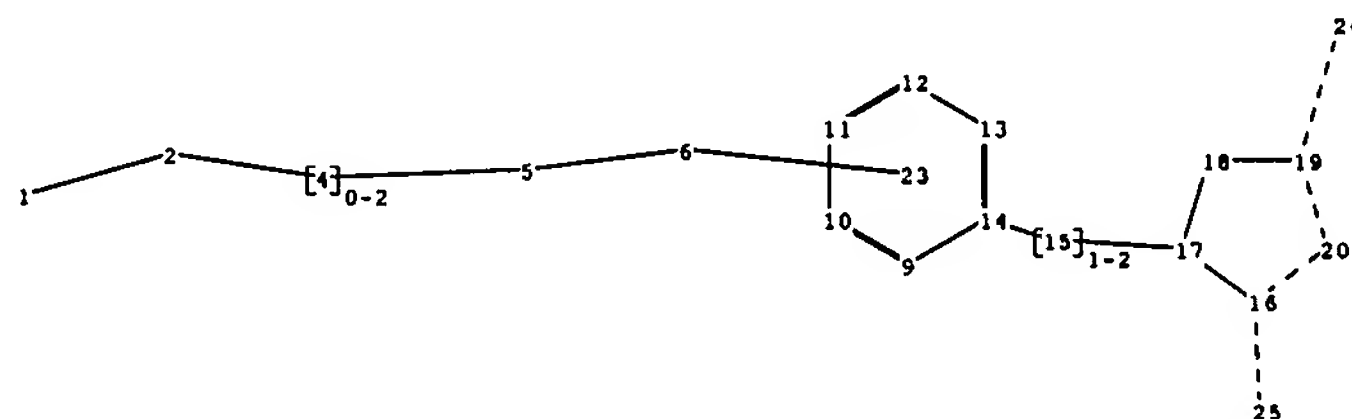
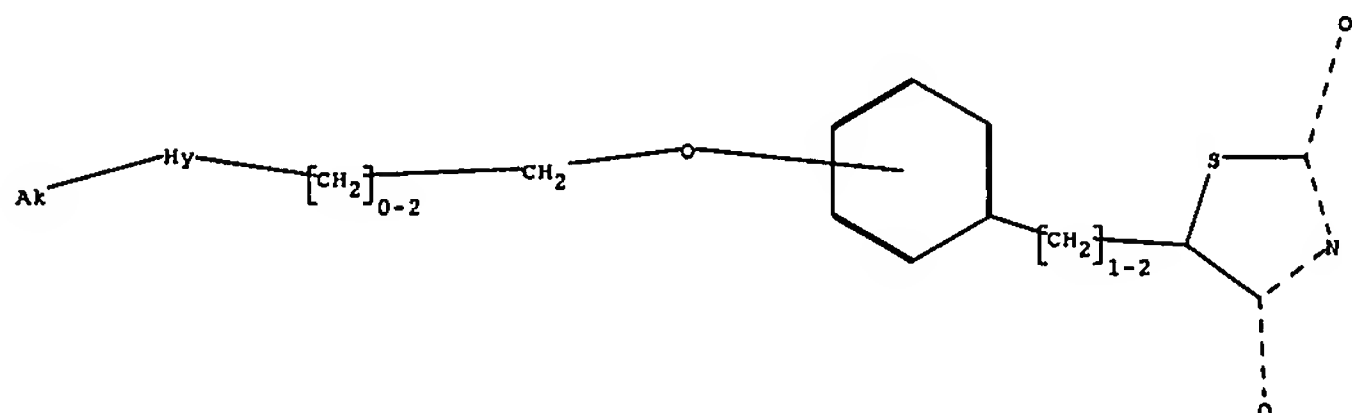
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 11:CLASS
12:CLASS



chain nodes :
 1 2 5 6 7 16 17 18 19
 ring nodes :
 10 11 12 13 14 15
 chain bonds :
 1-2 1-5 5-6 6-7 7-12 16-17 17-18 17-19
 ring bonds :
 10-11 10-15 11-12 12-13 13-14 14-15
 exact/norm bonds :
 1-2 1-5 7-12 17-19
 exact bonds :
 5-6 6-7 16-17 17-18
 normalized bonds :
 10-11 10-15 11-12 12-13 13-14 14-15
 isolated ring systems :
 containing 10 :

Connectivity :
 2:1 E exact RC ring/chain
 Match level :
 1:Atom 2:CLASS 5:CLASS 6:CLASS 7:CLASS 10:Atom 11:Atom 12:Atom
 13:Atom 14:Atom 15:Atom 16:CLASS 17:CLASS 18:CLASS 19:CLASS
 Generic attributes :
 1:
 Saturation : Unsaturated
 Number of Carbon Atoms : less than 7
 Number of Hetero Atoms : Exactly 1
 Type of Ring System : Monocyclic

Element Count :
 Node 1: Limited
 N,N1
 C,C5



chain nodes :

1 2 4 5 6 15 24 25

ring nodes :

9 10 11 12 13 14 16 17 18 19 20

chain bonds :

1-2 2-4 4-5 5-6 14-15 15-17 16-25 19-24

ring bonds :

9-10 9-14 10-11 11-12 12-13 13-14 16-17 16-20 17-18 18-19 19-20

exact/norm bonds :

1-2 2-4 16-20 16-25 19-20 19-24

exact bonds :

4-5 5-6 14-15 15-17 16-17 17-18 18-19

normalized bonds :

9-10 9-14 10-11 11-12 12-13 13-14

isolated ring systems :

containing 16 :

Match level :

1:CLASS 2:Atom 4:CLASS 5:CLASS 6:CLASS 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 23:Atom 24:CLASS 25:CLASS

Generic attributes :

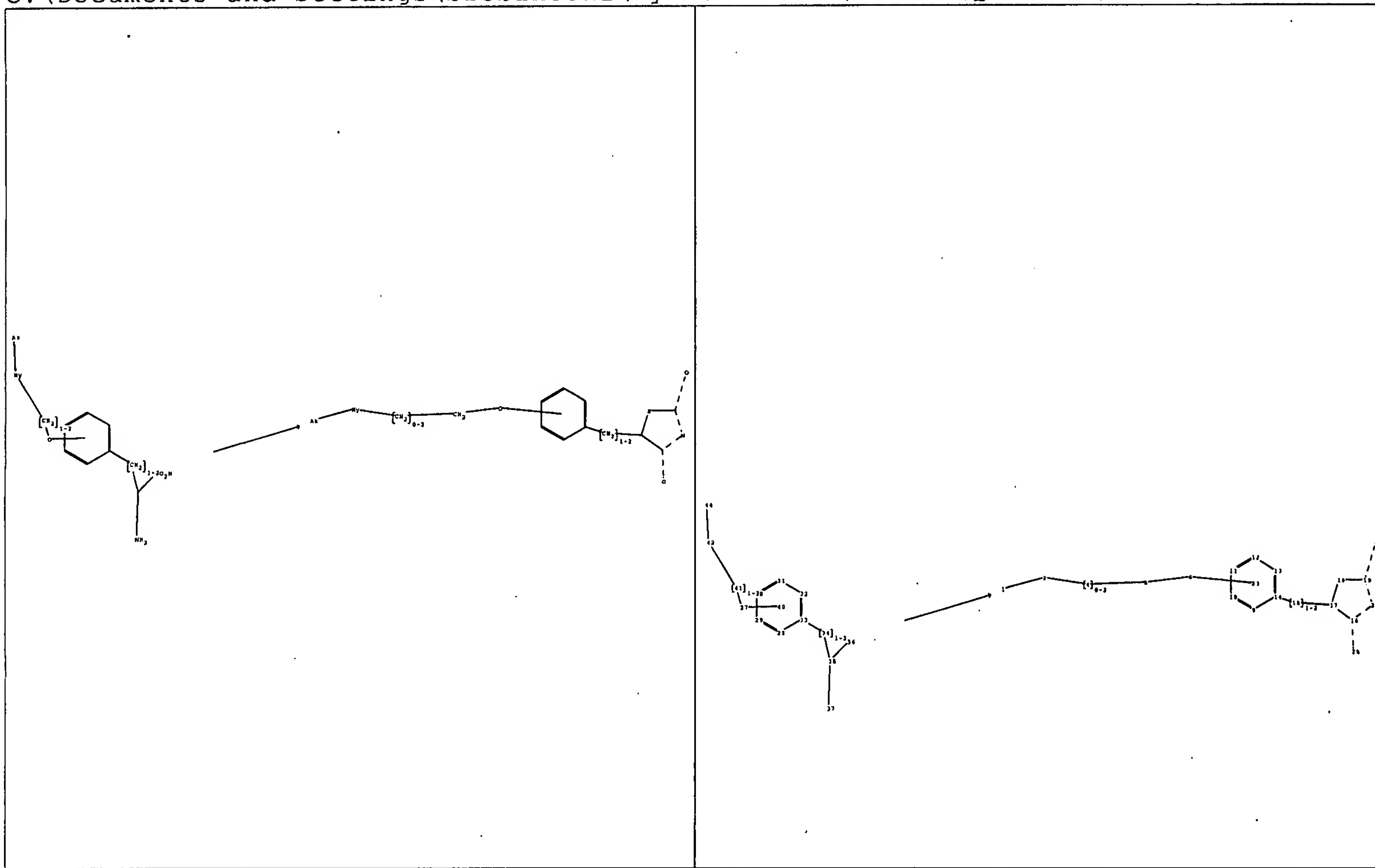
2:
Saturation : Unsaturated
Number of Carbon Atoms : less than 7
Number of Hetero Atoms : Exactly 1
Type of Ring System : Monocyclic

Element Count :

Node 2: Limited

N,N1

C,C5



chain nodes :

1 2 4 5 6 15 24 25 27 34 35 36 37 41 42 44

ring nodes :

9 10 11 12 13 14 16 17 18 19 20 28 29 30 31 32 33

chain bonds :

1-2 2-4 4-5 5-6 14-15 15-17 16-25 19-24 27-41 33-34 34-35 35-36
35-37 41-42 42-44

ring bonds :

9-10 9-14 10-11 11-12 12-13 13-14 16-17 16-20 17-18 18-19 19-20
28-29 28-33 29-30 30-31 31-32 32-33

exact/norm bonds :

1-2 2-4 16-20 16-25 19-20 19-24 35-37 41-42 42-44

exact bonds :

4-5 5-6 14-15 15-17 16-17 17-18 18-19 27-41 33-34 34-35 35-36

normalized bonds :

9-10 9-14 10-11 11-12 12-13 13-14 28-29 28-33 29-30 30-31 31-32
32-33

isolated ring systems :

containing 16 : 28 :

Connectivity :

44:1 E exact RC ring/chain

Match level :

1:CLASS 2:Atom 4:CLASS 5:CLASS 6:CLASS 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 23:Atom 24:CLASS 25:CLASS 27:CLASS 28:Atom 29:Atom 30:Atom
31:Atom 32:Atom 33:Atom 34:CLASS 35:CLASS 36:CLASS 37:CLASS 40:Atom
41:CLASS 42:Atom 44:CLASS

Generic attributes :

2:

Saturation : Unsaturated
Number of Carbon Atoms : less than 7
Number of Hetero Atoms : Exactly 1

Type of Ring System : Monocyclic
42:
Saturation : Unsaturated
Number of Carbon Atoms : less than 7
Number of Hetero Atoms : Exactly 1
Type of Ring System : Monocyclic

fragments assigned reactant role:
containing 27

fragments assigned product role:
containing 1

Element Count :

Node 2: Limited
N,N1
C,C5

Node 42: Limited
C,C5
N,N1